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# Project Summary

# Research on Numerical Transport Algorithms for Air Quality Simulation Models

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Errors introduced by advection schemes are considered to be an important source of inaccuracy in air quality models. Recently, significant research efforts focused on construction of advection schemes that yield highly accurate and oscillation-free solutions on a fixed grid system. Other requirements are also imposed on pollutant advection schemes such as mass conservation and positive solutions. Mass conservation is necessary to account accurately for pollutant mass balance. Preservation of positive concentrations is important because of the nonlinearity of atmospheric chemistry. There is no scheme, at present, that fully satisfies all of these requirements. For example, high accuracy usually comes at the expense of spurious oscillations, especially near steep gradients. The objective of this study is to identify advection schemes with more desirable properties for air quality modeling.

The performances of the following eight schemes are evaluated: (1) Smolarkiewicz' scheme, (2) piecewise parabolic method, (3) Bott's scheme, (4) Yamartino's scheme, (5) flux-corrected transport, (6) the semi-Lagrangian method, (7) chapeau function scheme, and (8) accurate space derivative scheme. The evaluation cases are selected from idealized problems with known analytic solutions. Problems relevant to air quality modeling are preferred such as one-dimensional advection with uniform velocity, rotation of a cone-shaped puff, skew advection of a point-source plume, shear flow tests and rotation of chemically reactive puffs. Quantitative measures are used in the evaluation so that properties of different schemes can be compared readily. Most schemes performed consistently in all the tests, but a few failed in some stressful tests. The differences between performances were more pronounced in some tests, and the ranking differed from test to test. However, important properties of the schemes were identified as a result of the diversity of the tests. Bott's, Yamartino's and accurate space derivative schemes are in general more accurate than the others. Bott's and Yamartino's schemes are computationally less demanding. Short-wavelength performance of Yamartino's scheme and its essentially oscillation free behavior compared to Bott's scheme are noteworthy.

*This Project Summary was developed by EPA's National Exposure Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).*

## Introduction

Modeling the fate of pollutants on urban and regional scales is a major research area for the U.S. EPA. Simulation of pollutant transport by the wind has been one of the focal research topics of the air quality modeling. We assume that the transport of pollutants in the atmospheric turbulent flow field can be described by means of differential equations and appropriate initial and boundary conditions. In Eulerian air quality models, the transport process is solved using appropriate numerical algorithms. These numerical algorithms for the advection processes must satisfy several properties that are

essential for making useful air quality simulations. As with all numerical methods, the numerical schemes for solving the transport equation must meet the convergence condition and correctly model the conservative, transportive, dissipative, and dispersive properties of the governing equation.

Due to the presence of pollutant sources and highly nonlinear chemical interactions between the concentration fields of different species, it is necessary to consider schemes with special properties: mass conservation, small numerical diffusion and small phase errors. Advection schemes with different properties introduce different errors, all of which are sources of uncertainty in air quality model predictions. It is critical to identify which of the above-mentioned properties a scheme possesses before recommending its use. Since an advection scheme with all the desired properties is not currently available, the issue becomes identifying the scheme with the most desirable properties and efficiency.

This report summarizes the work that was done under a cooperative agreement between the U.S. EPA and the MCNC-North Carolina Supercomputing Center. The objectives of the program were to study important numerical characteristics of various advection schemes, to test feasibility of their use in air quality simulations, and to show that the algorithms are capable of following accurately and efficiently pollutant transport. In this report, we describe desirable characteristics of eight one-dimensional numerical advection schemes currently used in air quality models. We evaluated these schemes by comparing a few quantitative measures obtained through several robust test cases relevant to air quality simulation. The numerical algorithm studied during the period of the project were incorporated into the pool of optional advection modules of the EPA's Models-3 Community Multiscale Air Quality (CMAQ) modeling system. The research findings from this project should be applicable to other regional/urban air quality models.

## Advection Algorithms

There are many different ways of classifying advection schemes. A common way is to classify the schemes based on the method used in their formulation. Since a wide variety of methods were used, any classification may fall short of being complete. The following is a fairly comprehensive list: (1) finite difference schemes, (2) finite volume schemes, (3) flux corrected schemes, (4) Lagrangian schemes, (5) finite element schemes, and (6) spectral schemes. Current trends in advection scheme development show a merging of the methods to take advantage of each approach's most desirable properties. For example, the Characteristic-Galerkin method combines the best of the finite element and Lagrangian methods. Flux corrections are being used in the framework of finite element and spectral schemes. Also, the classical finite difference schemes are being abandoned in favor of modern finite volume schemes. Eight advection schemes studied are listed below:

The Smolarkiewicz scheme (SMO) is based on the first-order accurate upstream or "donor cell" method. To increase accuracy, Smolarkiewicz reversed the effect of this artificial diffusion by defining an antidiffusion velocity. Though diffusion is physically irreversible, it is numerically possible to apply an antidiffusive step and partially recover what has been lost to diffusion; this resembles reversing a film that shows diffusion. It is customary to express the algorithm as a multistep scheme.

Bott scheme (BOT) uses normalized advective fluxes represented in polynomial form in an attempt to reduce the phase-speed errors. Negative values of the transported quantity are suppressed by nonlinearly limiting the normalized fluxes. Recently, a monotonic version of the scheme was developed and the time-splitting errors associated with the use of one-dimensional operators in multidimensional applications were reduced.

In the piecewise parabolic method (PPM), the subgrid distribution of the advected quantity is represented by a parabola in each grid interval. PPM not only provides a local fit of the data, but is monotonic and uses a special steepening procedure in the vicinity of sharp gradients. This ensures that positive quantities will remain positive and that sharp gradients will be handled correctly without the generation of spurious oscillations.

Yamartino scheme (YAM) uses piecewise cubic interpolands as a starting point for his higher-order scheme. In this scheme, the coefficients of a cell-centered cubic polynomial are constrained from the point of view of maintaining high-accuracy and low-diffusion characteristics while avoiding undesirable byproducts associated with higher-order schemes but absent in low-order schemes. In addition, a filter is used for filling in undesired short-wavelength minima. One advantage of Yamartino's scheme is that it was designed to follow short-wavelength features.

Flux-corrected transport (FCT) is a technique developed by Boris and Book. It constructs the net transportive flux as a weighted average of a flux computed by a low-order scheme and a flux computed by a higher-order scheme. The weighting is done in a manner that ensures that the higher-order flux is used to the greatest extent possible without introducing the overshoots and undershoots. Zalesak generalized FCT to multidimensions.

In a semi-Lagrangian method (SLT), one estimates the backward trajectory of a particle that arrives at a certain grid point. Since the origin of a particle does not always coincide with a grid point, an interpolation scheme is necessary to estimate the original concentration. Once estimated, this concentration is assigned to the grid point of arrival. One advantage of the scheme is that it is not subject to the Courant stability condition, so large time steps can be used.

The accurate space derivative (ASD) scheme is based on a pseudo-spectral method. This scheme is highly accurate; however, it needs to be coupled with a nonlinear filter (such as the Forester filter) to suppress the spurious oscillations that may exist in the solution. A disadvantage of the scheme is the requirement of periodic boundary conditions inherent to all spectral schemes.

The chapeau function method (HAT) is a classical weighted-residual finite element method. The solution is expanded in piecewise basis functions that look like hats ("chapeau" is French for hat) in one-dimensional space: Then the residual is assumed to be orthogonal to the weighting functions, which may be the basis functions themselves, as is usually the case in the Bubnov-Galerkin methods.

## Results and Discussion

Eight advection schemes (not counting the variations of Bott Scheme) were compared using test cases ranging from very simple one-dimensional advection to more robust two-dimensional shear and chemically reactive flows. Most schemes performed consistently in all the tests, but a few failed in some stressful tests. The differences between performances were more pronounced in some tests, and the ranking differed from test to test. However, important properties of the schemes were identified as a result of the diversity of the tests. This preliminary testing of the schemes resulted in the following findings:

- ASD has very high accuracy but is not strictly mass conservative. It is

not monotonic but usually yields a positive result.

- BOT is highly accurate and mass conservative. It may create ripples and overshoots, but it is positive-definite.

- FCT is fairly accurate and mass conservative. It does not create any ripples or overshoots, but does so at the expense of diffusion to the background.

- HAT has fair accuracy and is mass conservative. However, it may lead to ripples that can grow and cause instabilities.

- PPM also has good accuracy and is strictly mass conservative and monotonic. While the diffusion to the background is very small, peak clipping can be significant.

- SLT has poor accuracy and severe mass conservation problems. The only positive feature of SLT is that it does not lead to ripples.

- SMO has relatively low accuracy. It is mass conservative but it may lead to ripples in concentration fields.

- YAM has very high accuracy even for the shortest wavelengths, and is mass conservative. It can lead to overshoots under certain situations.

In addition to the properties discussed above, the computational performances of the schemes were also considered in the ranking. The CPU times for all the tests were averaged and normalized with respect to SMO. The only scheme that is less CPU intensive than SMO is BOT; other schemes require more CPU time. ASD is the most CPU-intensive scheme: it requires more than four times more CPU than SMO does.

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